

TEST FUNCTION SPACES FOR GEOMETRIC FINITE ELEMENTS

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ABSTRACT. We construct test function spaces for geometric finite elements. Geometric finite elements (GFE) are generalizations of Lagrangian finite elements to situations where the unknown function maps into a nonlinear space. Test functions for such spaces arise as variations of GFE functions wherever the GFE function space has a local manifold structure. For any given GFE function u_h , the test functions form a linear space that depends on u_h . They generalize Jacobi fields in the same way that the GFE interpolation functions generalize geodesic curves. Having test function spaces allows to extend the GFE method to boundary value problems that do not have a minimization formulation.

Keywords: geometric finite elements, geodesic interpolation, projection-based interpolation, test functions, generalized Jacobi fields

1. INTRODUCTION

Geometric finite elements (GFE) are generalizations of Lagrangian finite elements that discretize spaces of maps into a nonlinear Riemannian manifold M . The classical Lagrangian finite element functions are recovered when $M = \mathbb{R}$. The generalizations can be achieved in a number of ways. Originally, *geodesic* finite elements were introduced for one-dimensional, first-order approximations [14], and subsequently generalized to domains of arbitrary dimension [15], and higher approximation orders [17]. Optimal discretization error bounds were proved in [4, 5], and the discretization has been applied successfully to problems in Cosserat mechanics [14, 18] and the computations of harmonic maps [17]. Later, *projection-based* finite elements were proposed and investigated in [3, 20].

In all these publications, geometric finite elements have only been applied to problems with a minimization formulation. The fact that GFE functions are H^1 maps allowed to reformulate the energy formulations straightforwardly as minimization problems for algebraic functionals defined on a product manifold M^n , with n the number of Lagrange nodes of the grid. Variations and optimality were only considered in this algebraic setting.

However, even though this does not directly follow from the original publications, GFE can also be used for problems without a minimization structure. The missing ingredient for this are spaces of suitable test functions. In this short note we construct such spaces. Their definition follows directly from the local manifold structure of the discrete space, and they generalize the Jacobi fields of classical differential geometry (e.g., [8, Chap. 5]). As such, they form linear spaces of vector fields along GFE functions, and these spaces can be identified with their values at

the Lagrange nodes. Disregarding a few minor technical differences, the construction is the same both for geodesic finite elements and for projection-based finite elements.

The construction of test functions as variations will appear trivial to people with experience in geometric analysis. On the other hand, for people with a numerical analysis background this construction may not be quite as clear, and the author has been prompted to write this article by repeated questions about the existence and nature of GFE test functions.

Evaluating GFE test functions is easy and cheap. For geodesic finite elements, provided the value of a GFE function $u_h : \Omega \rightarrow M$ is given at a point x , then evaluating a test function for u_h at the same point involves only solving one linear system of equations in $\dim M$ variables. For projection-based finite elements, the evaluation procedure depends on how the projection onto M from an embedding space can be computed. For the important case of M being a sphere, there is even a closed-form expression for the test functions.

Having test functions allows to state optimality conditions for minimization problems directly in GFE spaces, in contrast to the approach of [15, 17], which formulated optimality conditions only in the algebraic setting. We work out both approaches, and show in Section 4 by trivial computations that both are equivalent. This otherwise obvious result justifies our construction.

2. GEOMETRIC FINITE ELEMENTS

We briefly review the two main constructions of geometric finite elements. These differ only in the way Lagrange interpolation on a single element is generalized to nonlinear spaces. The first approach, geodesic interpolation, is completely intrinsic. Alternatively, projection-based interpolation needs an embedding space of M , but leads to more efficient algorithms for certain choices of M .

2.1. Sobolev spaces of manifold-valued functions. Let Ω be an open and connected subset of \mathbb{R}^d with a Lipschitz boundary, and let M be a smooth, connected manifold. The following definition of a Sobolev space for functions with values in M is standard (see, e.g., [5, 19]).

Definition 2.1. Let $\iota : M \rightarrow \mathbb{R}^N$ be an isometric embedding (which always exists by [11]). For $k \in \mathbb{N}_0$ and $p \in \mathbb{N} \cup \{\infty\}$ define

$$W^{k,p}(\Omega, M) := \{v \in W^{k,p}(\Omega, \mathbb{R}^N) : v(x) \in \iota(M), \text{ a.e.}\}.$$

For nonlinear M these spaces obviously do not form vector spaces. However, under certain smoothness conditions the manifold structure of M is inherited. The following result is proved in [13].

Lemma 2.1. If $k > d/p$, the spaces $W^{k,p}(\Omega, M)$ are Banach manifolds.

The GFE method is a way to discretize such nonlinear function spaces. Its central idea are generalizations of Lagrange interpolation to interpolation of values given on a nonlinear manifold.

2.2. Geodesic interpolation. The first approach to interpolation of values on M is completely intrinsic. Let T_{ref} be a bounded domain in \mathbb{R}^d , with coordinates ξ . We call T_{ref} a reference element. On its closure \bar{T}_{ref} we have a set of distinct Lagrange nodes $a_i, 1 \leq i \leq m$, and corresponding scalar Lagrangian interpolation functions

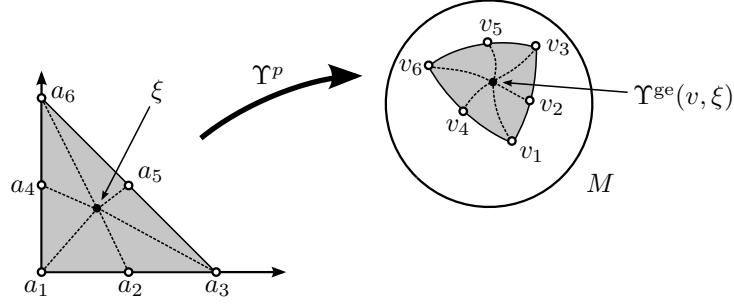


FIGURE 1. Second-order geodesic interpolation from the reference triangle into a sphere

$\varphi_1, \dots, \varphi_m$, i.e., p -th order polynomial functions with $\varphi_i(a_j) = \delta_{ij}$. We assume that the φ_i and a_i are such that the corresponding interpolation problem is well posed, i.e., for given $v_i \in \mathbb{R}$, $i = 1, \dots, m$ there is a single function $\pi : T_{\text{ref}} \rightarrow \mathbb{R}$ in the span of the φ_i such that $\pi(a_i) = v_i$ for all $1 \leq i \leq m$.

We want to construct a function $\Upsilon^{\text{ge}} : T_{\text{ref}} \rightarrow M$ that interpolates a given set of values $v_1, \dots, v_m \in M$. The following definition has been given in [17] and [2]. It is visualized in Figure 1.

Definition 2.2. Let $T_{\text{ref}} \subset \mathbb{R}^d$ be a bounded domain, and M a connected, smooth, complete manifold with a distance metric $\text{dist}(\cdot, \cdot) : M \times M \rightarrow \mathbb{R}$. Let $\varphi_1, \dots, \varphi_m$ be a set of p -th order scalar Lagrangian shape functions, and let $v = (v_1, \dots, v_m) \in M^m$ be values at the corresponding Lagrange nodes. We call

$$\begin{aligned} \Upsilon^{\text{ge}} &: M^m \times T_{\text{ref}} \rightarrow M \\ \Upsilon^{\text{ge}}(v, \xi) &:= \arg \min_{q \in M} \sum_{i=1}^m \varphi_i(\xi) \text{dist}(v_i, q)^2 \end{aligned}$$

p -th order geodesic interpolation on M . For given T_{ref} , a_1, \dots, a_m , and $\varphi_1, \dots, \varphi_m$, the space of all such functions will be denoted by $P_p^{\text{ge}}(M)$.

We will look at the functions Υ^{ge} sometimes as functions of ξ or of the v_1, \dots, v_m only, and adapt our notation accordingly. The meaning should always be clear from the context.

As values of Υ^{ge} are minimizers of a functional

$$(1) \quad f_{v, \xi}(q) := \sum_{i=1}^m \varphi_i(\xi) \text{dist}(v_i, q)^2,$$

they fulfill a first-order optimality criterion. For any $q \in M$, let \log_q be the inverse of the exponential map of M at q . Then, we have

$$(2) \quad \sum_{i=1}^m \varphi_i(\xi) \log_{\Upsilon^{\text{ge}}(v, \xi)} v_i = 0,$$

provided the quantities are close enough to each other so that \log is defined [9, Thm. 1.2].

Important properties, like C^∞ -differentiability of Υ^{ge} with respect to all of its arguments, have been shown in [15, 17]. Of central importance for the construction

of test functions is the well-posedness of the definition, which holds if the nodal values v_1, \dots, v_m are “close together” in a certain sense. The precise conditions for first-order functions have been given by Karcher [9]. Remember that a set $D \subset M$ is called convex if for each $p, q \in D$ the minimizing geodesic from p to q is entirely contained in D .

Theorem 2.1 (Karcher [9]). *Let M be complete, $\varphi_1, \dots, \varphi_m$ a first-order scalar Lagrange basis on a reference element T_{ref} , B_ρ an open convex geodesic ball of radius ρ in M , and $v_1, \dots, v_m \in B_\rho$.*

- (1) *If the sectional curvatures of M in B_ρ are bounded by a positive constant K , and $\rho < \frac{1}{4}\pi K^{-1/2}$, then the function $f_{v,\xi}$ defined in (1) has a unique minimizer in B_ρ for all $\xi \in T_{\text{ref}}$.*
- (2) *If the sectional curvatures of M in B_ρ are at most 0, then $f_{v,\xi}$ has a unique minimizer in B_ρ for all $\xi \in T_{\text{ref}}$.*

Different arguments are needed to show corresponding results for Lagrange polynomials φ_i of order 2 and higher, because such polynomials can take negative values. A simple proof for the following qualitative result is given in [5]. A more quantitative result appears in [17].

Theorem 2.2. *Let M be complete, and $\varphi_1, \dots, \varphi_m$ a scalar Lagrange basis on T_{ref} . Let $B_D \subset B_\rho$ be two concentric geodesic balls in M of radii D and ρ , respectively. There are numbers D and ρ such that if the values v_1, \dots, v_m are contained in B_D , then the function $f_{v,\xi}(q)$ defined in (1) has a unique minimizer in B_ρ .*

2.3. Projection-based interpolation. An alternative generalization of Lagrange interpolation uses embedding spaces and projections. Let again $\iota : M \rightarrow \mathbb{R}^N$ be an isometric embedding, and let $\mathcal{P} : \mathbb{R}^N \supset U \rightarrow M$ be a projection from a neighborhood U of $\iota(M)$ onto M . Let T_{ref} , a_i , φ_i , and v_i , $i = 1, \dots, m$, be as in the previous section. Then we can interpolate between the values v_i by first interpolating in the embedding space, and then projecting pointwise onto M .

Definition 2.3 ([3, 20]). *Let $T_{\text{ref}} \subset \mathbb{R}^d$ be a bounded domain, M a connected manifold with an embedding $\iota : M \rightarrow \mathbb{R}^N$, and let \mathcal{P} be a projection from a neighborhood U of $\iota(M)$ onto M . Let $\varphi_1, \dots, \varphi_m$ be a set of p -th order scalar Lagrangian shape functions, and let $v = (v_1, \dots, v_m) \in M^m$ be values at the corresponding Lagrange nodes. We call*

$$\Upsilon^{pr} : M^m \times T_{\text{ref}} \rightarrow M$$

$$(3) \quad \Upsilon^{pr}(v, \xi) := \mathcal{P} \left[\sum_{i=1}^m \varphi_i(\xi) \iota(v_i) \right]$$

projection-based interpolation on M . For given T_{ref} and $\varphi_1, \dots, \varphi_m$, the space of all such functions will be denoted by $P_p^{pr}(M)$.

Like geodesic interpolation, projection-based interpolation is usually not defined for all combinations of values $v_1, \dots, v_m \in M$. The reason is that it is frequently impossible to define continuous projections \mathcal{P} onto M on all of \mathbb{R}^N . The intuition that interpolation is well-defined if the v_1, \dots, v_m are close to each other still holds, but no more precise results are currently available.

Sprecher showed in [20] that projection-based interpolation can be interpreted as geodesic interpolation if M is equipped with the distance metric of the Euclidean embedding space.

Lemma 2.2 ([20, Prop. 1.4.4]). *Let \mathcal{P} be the closest-point projection from \mathbb{R}^N onto M . With the notation of Definitions 2.2 and 2.3 we have*

$$\Upsilon^{\text{pr}}(v, \xi) := \mathcal{P} \left[\sum_{i=1}^m \varphi_i(\xi) \iota(v_i) \right] = \arg \min_{q \in M} \sum_{i=1}^m \varphi_i(\xi) \|\iota(v_i) - \iota(q)\|^2.$$

Nevertheless, the direct definition (3) is advantageous if an easily computable \mathcal{P} is available. In that case, (3) is a straightforward way to compute the interpolation function, unlike the implicit construction used in Definition 2.2. Also, it is quite obvious from (3) that Υ^{pr} is differentiable whenever \mathcal{P} is, which is more difficult to show for geodesic interpolation.

Useful embeddings are available for a number of important spaces. If M is the unit sphere, \mathcal{P} is easily evaluated as

$$\mathcal{P}(w) = \frac{w}{\|w\|}.$$

The interpolation polynomial Υ^{pr} is then well-defined unless $\sum_{i=1}^m \varphi_i(\cdot) \iota(v_i)$ has a zero. The derivative of Υ^{pr} with respect to ξ is

$$\frac{\partial}{\partial \xi} \Upsilon^{\text{pr}}(v, \xi) = \frac{\partial \mathcal{P}(w)}{\partial w} \Big|_{w=\sum_{i=1}^m \varphi_i(\xi) \iota(v_i)} \cdot \sum_{i=1}^m \frac{\partial \varphi_i}{\partial \xi} \iota(v_i),$$

where

$$\frac{\partial \mathcal{P}(w)}{\partial w} = I \|w\|^{-1} - ww^T \|w\|^{-3}.$$

For the special orthogonal group $\text{SO}(N) \subset \mathbb{R}^{N \times N}$, the closest-point projection in the Frobenius norm is the polar decomposition [12]. Closed-form expressions for the polar factor of a given matrix A exist [7], but it is more convenient to compute it and its derivatives through the iteration defined by $Q_0 := A$ and

$$Q_{k+1} := \frac{1}{2} (Q_k + Q_k^{-T}),$$

which converges quadratically to the polar factor of A [6]. Alternatively, one may consider different projections like Gram–Schmidt orthogonalization or QR decomposition.

Some manifolds like the set of all symmetric positive definite $N \times N$ matrices form open subsets of Euclidean spaces. In such a case no natural projection is available.

2.4. Global geometric finite element spaces. Given an interpolation rule from one of the two previous sections, it is easy to construct global finite element spaces. Most of what follows in the rest of this paper is independent of whether geodesic or projection-based interpolation is used. We write Υ to mean either one of Υ^{ge} and Υ^{pr} , and P_p for the corresponding spaces of generalized polynomials.

Let Ω be an open bounded subset of \mathbb{R}^d , $d \geq 1$. For simplicity we assume that Ω has a polygonal boundary. Let \mathcal{G} be a conforming grid for Ω with elements of arbitrary type. We denote by $x_i \in \Omega$, $i = 1, \dots, n$ the union of the sets of Lagrange nodes of the individual elements.

Definition 2.4 (Geometric finite elements [15, 17, 20]). *We call $v_h : \Omega \rightarrow M$ a p -th order geometric finite element function if it is continuous, and if for each element*

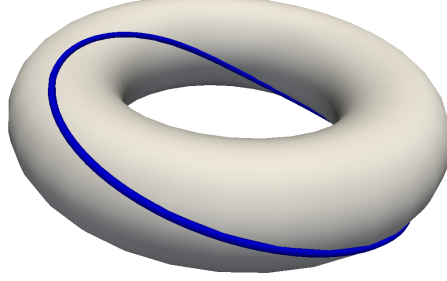


FIGURE 2. Illustration of the global structure of the simple-most GFE space. Let $\Omega = [0, 1]$ be discretized by a single element, set $p = 1$ and $M = S^1$. Then the algebraic configuration space is $S^1 \times S^1$, which is isomorphic to a torus in \mathbb{R}^3 . The discrete space $V_h^{S^1}$ is isomorphic to that torus, except for all configurations $(v_1, v_2) \in S^1 \times S^1$ with $v_1 = -v_2$. For each such configuration, there are two geodesic FE functions interpolating the values v_1 and v_2 , and hence the torus has two “sheets” there. On the other hand, no projection-based interpolation exists for these configurations at all. The problematic configurations form a closed path which circles once around the torus, illustrated by the blue line.

$T \in \mathcal{G}$ the restriction $v_h|_T$ is a p -th order geometric interpolation in the sense that

$$v_h|_T(x) = \Upsilon(v_{T,1}, \dots, v_{T,m}; \mathcal{F}_T(x)),$$

where $\mathcal{F}_T : T \rightarrow T_{\text{ref}}$ is affine or multilinear, T_{ref} is the reference element corresponding to T , and the $v_{T,i}$ are values in M . The space of all such functions v_h (for a fixed p) will be denoted by V_h^M .

Geometric finite element functions are Sobolev functions in the sense of Definition 2.1. The following conformity result was shown in [15].

Theorem 2.3. $V_h^M(\Omega) \subset H^1(\Omega, M)$.

We now briefly discuss aspects of the global structure of the set V_h^M . Partial results can be obtained by using its relationship to the product space $M^n := \prod_{i=1}^n M$ (the “algebraic” space). However, the relationship between geometric finite element functions $v_h \in V_h^M$ and sets of coefficients $\bar{v} \in M^n$ is more subtle than in the linear case, where the two are isomorphic to each other. The problem is that the coefficients may be such that the interpolation problem is not well posed on all grid elements. We try to illustrate this effect in Figure 2 for $M = S^1$, $d = 1$, $p = 1$, with a grid \mathcal{G} consisting of a single element. Here, the algebraic space is the torus $S^1 \times S^1$, but the corresponding GFE space $V_h^{S^1}$ is larger if geodesic interpolation is used, and smaller for projection-based interpolation.

To formally investigate the relationship we define the nodal evaluation operator

$$\begin{aligned} \mathcal{E} : V_h^M &\rightarrow M^n \\ (\mathcal{E}(v_h))_i &= v_h(x_i), \quad x_i \text{ the } i\text{-th Lagrange node of } \mathcal{G}. \end{aligned}$$

To each geometric finite element function $v_h \in V_h^M$ it associates the set of function values at the Lagrange nodes. Since functions in V_h^M are continuous, the operator \mathcal{E} is well-defined and single-valued for all $v_h \in V_h^M$.

For traditional finite elements with values in a linear space, the evaluation operator is an isomorphism. In particular, its inverse \mathcal{E}^{-1} , which associates finite element functions to a given set of coefficients, exists everywhere, and is single-valued. This does not hold for geometric finite elements. For arbitrary $\bar{v} \in M^n$, the operator \mathcal{E}^{-1} may be multi-valued, or may not exist at all. For geodesic interpolation, Theorem 2.2 allows to characterize the sets of coefficients for which \mathcal{E}^{-1} is single-valued. See [17] for details.

However, the algorithmic treatment of finite element functions can only work by manipulating an algebraic representation of finite element functions. We therefore restrict our attention to the set where \mathcal{E}^{-1} is defined and single-valued

$$\widetilde{\mathcal{M}} := \{\bar{v} \in M^n : \mathcal{E}^{-1} \text{ is defined and single-valued at } \bar{v}\}.$$

It is currently an open problem whether the set $\widetilde{\mathcal{M}}$ is open. To be able to argue with manifold properties of the algebraic space, we restrict our attention even further, to the interior of $\widetilde{\mathcal{M}}$

$$\mathcal{M} := \text{int } \widetilde{\mathcal{M}}.$$

As an open subset of a manifold, \mathcal{M} is a manifold itself. It is unclear whether \mathcal{M} is connected, but we will not use connectedness. However, for geodesic interpolation the following theorem shows that \mathcal{M} has a nonempty interior, if the grid is fine enough.

Theorem 2.4 ([17]). *Let M be a Riemannian manifold, and let $v : \Omega \rightarrow M$ be Lipschitz continuous in the sense that there exists a constant L such that*

$$\text{dist}(v(x), v(y)) \leq L\|x - y\|$$

for all $x, y \in \Omega$. Let \mathcal{G} be a grid of Ω and h the length of the longest edge of \mathcal{G} . Let \mathcal{E}^{ge} be the evaluation operator of geodesic finite elements. Let \bar{v} be the set of value of v at the Lagrange nodes. For h small enough, the inverse of \mathcal{E}^{ge} has only a single value in V_h^M for each $\bar{v} \in M^n$ in a neighborhood of \bar{v} .

Similar results can be shown for projection-based interpolation. They imply that for a given problem with a Lipschitz-continuous solution we can always find a grid fine enough such that we can disregard the distinction between V_h^M and M^n in the vicinity of the solution. Hence locally a geometric finite element problem can be represented by a corresponding algebraic problem on the product manifold M^n . In numerical experiments, this requirement of locality does not appear to pose a serious obstacle.

Locally around functions where Theorem 2.4 applies, the function space V_h^M inherits the differentiable manifold structure of $\mathcal{M} \subset M^n$, because functions defined by geodesic or projection-based interpolation depend differentiably on their corner values [17, Thm. 4.1]. In an abuse of notation, we will treat V_h^M as a manifold itself.

3. TEST FUNCTION SPACES

To motivate our construction of test functions we briefly revisit the theory of linear elliptic partial differential equations. Consider the linear reaction–diffusion equation

$$-\Delta u + u = f \quad \text{on } \Omega,$$

for a given function $f \in L^2(\Omega)$. The weak formulation is

$$(4) \quad a(u, v) = (f, v)_{L^2(\Omega)},$$

where

$$a(w, v) := \int_{\Omega} \nabla w \nabla v \, dx + \int_{\Omega} wv \, dx$$

is a bilinear form on $H^1(\Omega)$. Of its two arguments, the second one is called a *test function*.

The test function v is to be interpreted as a small variation around w . Indeed, solutions of (4) are minimizers of the functional

$$\mathcal{J} : H^1(\Omega) \rightarrow \mathbb{R}, \quad \mathcal{J}(w) := \frac{1}{2}a(w, w) - (f, w).$$

Local minimizers of \mathcal{J} are characterized by the directional derivative of \mathcal{J} being zero in all directions. The directional derivative of \mathcal{J} at a point $w \in H^1$ in the direction of a function v is

$$\frac{d\mathcal{J}(w)}{dv} = a(w, v) - (f, v)_{L^2(\Omega)}.$$

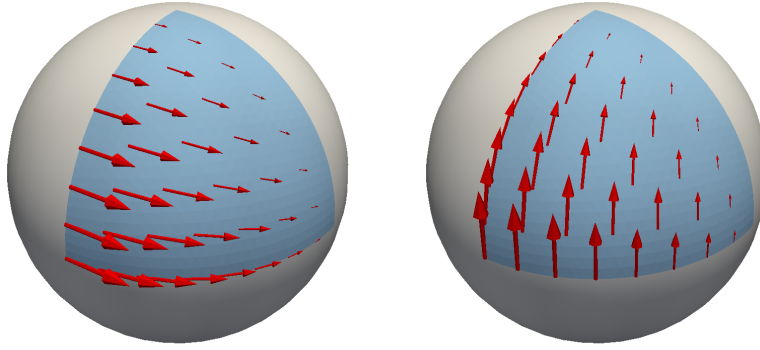
Hence the test function v in (4) can be interpreted as a direction vector based at u .

If we now consider functionals defined on a manifold \mathcal{N} , then small variations of a function $u \in \mathcal{N}$ are the elements of the tangent space $T_u\mathcal{N}$ of \mathcal{N} at u . There is not a single test function space anymore; rather, each configuration $u \in \mathcal{N}$ has its own test function space. Note, though, that for each $u \in \mathcal{N}$, the corresponding test functions form a linear space.

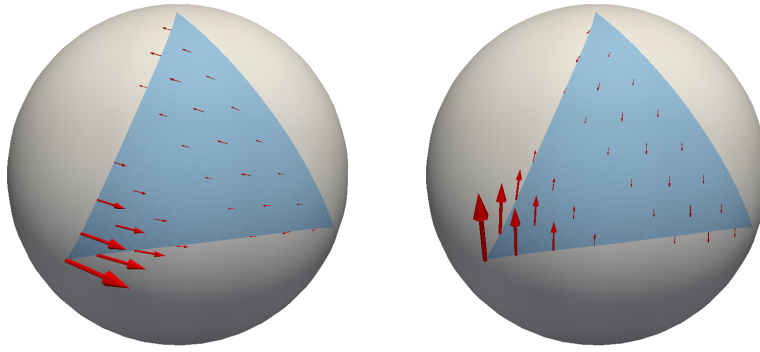
This construction is no contradiction to the linear theory, which takes u and v from the same space $H^1(\Omega)$. Indeed, if u is element of the space $H^1(\Omega)$ (which, for the sake of the intuitive argument here, we interpret as a manifold), then the test functions v must be chosen from the tangent space $T_u H^1(\Omega)$ of $H^1(\Omega)$ at u . However, since $H^1(\Omega)$ is a linear space, all its tangent spaces are isomorphic to the base space $H^1(\Omega)$. Therefore, claiming that the test functions must be from $H^1(\Omega)$ itself is merely an abuse of notation.

3.1. Generalized Jacobi fields. Motivated by the previous discussion, we construct test functions as tangent vectors to the GFE manifold V_h^M . We use the fact that a tangent vector η at a given point $u_h \in V_h^M$ is the derivative of a differentiable curve through u_h .

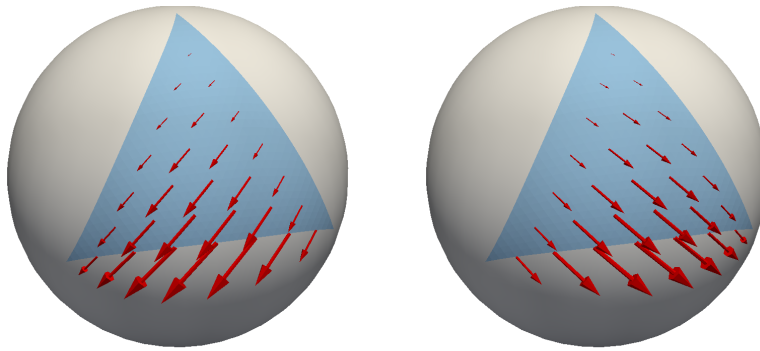
As for the construction of the GFE spaces themselves, we construct test functions first for interpolation functions on a reference element, and then piece them together to form global spaces.



(A) First-order



(B) Second-order, vertex degree of freedom



(C) Second-order, edge degree of freedom

FIGURE 3. Test functions along geodesic interpolation functions from a triangle into the sphere S^2 . These vector fields correspond to the shape functions normally used for Lagrangian finite element methods, because they are zero on all but one Lagrange point. Note how the second-order vertex vector fields in the second row partially point “backwards”, because the corresponding scalar shape functions have negative values on parts of their domains.

Definition 3.1. Let $\Upsilon \in P_p(M)$ be a geometric interpolation function for the values $v_1, \dots, v_m \in M$. A vector field η along Υ is called a variation of Υ , if there is a differentiable curve $c : (-\epsilon, \epsilon) \rightarrow P_p(M)$ such that

$$\dot{c}|_{t=0}(\xi) = \eta(\xi)$$

for all $\xi \in T_{\text{ref}}$.

Figure 3 shows six such vector fields along functions from $P_1^{\text{ge}}(S^2)$ and $P_2^{\text{ge}}(S^2)$, mapping the reference triangle to the unit sphere.

Definition 3.1 generalizes the well-known Jacobi fields, because if T_{ref} is one-dimensional, then a first-order geodesic interpolation Υ^{ge} is a geodesic curve between the Lagrange values [15, Lem. 2.2], and the variations constructed in Definition 3.1 are Jacobi fields [8, Thm. 5.2.1]. If, on the other hand, we set $M = \mathbb{R}$, the standard Lagrangian shape functions are obtained. Hence, Definition 3.1 is a direct generalization of the test functions normally used in the finite element method.

GFE test functions have an algebraic representation. Unlike for GFE functions themselves, where the relationship between discrete functions and algebraic representations is complicated, for test functions the two are isomorphic again.

Lemma 3.1. Let Υ be a geometric interpolation function for the values $v_1, \dots, v_m \in M$. The generalized Jacobi fields on Υ form a vector space \mathcal{V}_Υ , which is isomorphic to $\prod_{i=1}^m T_{v_i}M$. The isomorphism has an explicit representation as

$$\begin{aligned} \mathcal{T} : \prod_{i=1}^m T_{v_i}M &\rightarrow \mathcal{V}_\Upsilon \\ \mathcal{T}[b_1, \dots, b_m](\xi) &= \sum_{i=1}^m \frac{\partial \Upsilon(v_1, \dots, v_m; \xi)}{\partial v_i} \cdot b_i \end{aligned}$$

for all $b_i \in T_{v_i}M$, $i = 1, \dots, m$, and $\xi \in T_{\text{ref}}$.

Proof. Let η be a generalized Jacobi field along Υ . By definition, there is a curve c in $P_p(M)$ such that $\dot{c}(0) = \eta$. Let $C : (-\epsilon, \epsilon) \rightarrow M^m$ be the corresponding curve of point values at the Lagrange nodes. Then, the value of η at a point $\xi \in T_{\text{ref}}$ is

$$\begin{aligned} \eta(\xi) &= \dot{c}(\xi)|_{t=0} \\ &= \frac{d}{dt} \Upsilon(C(t), \xi) \Big|_{t=0} \\ &= \sum_{i=1}^m \frac{d}{dv_i} \Upsilon(C(0), \xi) \cdot \frac{dC_i(t)}{dt} \Big|_{t=0} \\ &= \mathcal{T}[b_1, \dots, b_m](\xi), \end{aligned}$$

with $b_i = \frac{dC_i(t)}{dt} \Big|_{t=0}$, $i = 1, \dots, m$. Hence there is a set of tangent vectors b_1, \dots, b_m such that $\mathcal{T}[b_1, \dots, b_m] = \eta$, and therefore \mathcal{T} is surjective.

On the other hand, the restriction of the vector field $\mathcal{T}[b_1, \dots, b_m]$ to the Lagrange nodes a_1, \dots, a_m yields b_1, \dots, b_m , since $\frac{\partial \Upsilon(a_j)}{\partial v_i}$ is the identity if $i = j$, and zero otherwise. Therefore \mathcal{T} is injective.

Finally, the linearity of \mathcal{T} follows from the linearity of the derivatives $\frac{\partial \Upsilon(v_1, \dots, v_m; \xi)}{\partial v_i}$. \square

The quantities $\frac{\partial \Upsilon}{\partial v_i}$ appearing in the expression for the isomorphism \mathcal{T} between coefficient vectors and vector fields are not new. They already appear in the expressions for the derivatives of energy functionals $J : M^n \rightarrow \mathbb{R}$ with respect to coefficients; for gradient descent and Newton-type methods. Computation is straightforward if Υ is projection-based interpolation with an explicitly given projection \mathcal{P} . For geodesic finite elements, it was later argued in [17, 18] that energy gradients and Hessians are best evaluated with an automatic differentiation system (and the same argument holds for projection-based finite elements as well). But a simple way to evaluate $\frac{\partial \Upsilon}{\partial v_i}$ for geodesic interpolation has been proposed in the literature nevertheless [15, 16], which we briefly revisit here.

Let $\Upsilon^{\text{ge}}(v, \xi) : M^m \times T_{\text{ref}} \rightarrow M$ be a function given by geodesic interpolation, $v_i \in M$, $i = 1, \dots, m$ the coefficients corresponding to the m Lagrange nodes, and let $\xi \in T_{\text{ref}}$ be arbitrary but fixed. We want to compute the derivatives

$$\frac{\partial}{\partial v_i} \Upsilon^{\text{ge}}(v_1, \dots, v_m; \xi) : T_{v_i} M \rightarrow T_{\Upsilon^{\text{ge}}(v, \xi)} M$$

for all $i = 1, \dots, m$. For this, we recall that values q^* of Υ^{ge} are minimizers of the functional

$$f_{v, \xi} : M \rightarrow \mathbb{R} \quad f_{v, \xi}(q) := \sum_{i=1}^m \varphi_i(\xi) \text{dist}(v_i, q)^2.$$

Hence, they fulfill the first-order optimality condition

$$F(v_1, \dots, v_m; \xi, q^*) := \left. \frac{\partial f_{v, \xi}(q)}{\partial q} \right|_{q=q^*} = 0.$$

Taking the derivative of this with respect to any of the v_i gives, by the chain rule,

$$\frac{dF}{dv_i} = \frac{\partial F}{\partial v_i} + \frac{\partial F}{\partial q} \cdot \frac{\partial \Upsilon^{\text{ge}}(v, \xi)}{\partial v_i} = 0,$$

with

$$(5) \quad \frac{\partial F}{\partial v_i} = \varphi_i(\xi) \frac{\partial}{\partial v_i} \frac{\partial}{\partial q} \text{dist}(v_i, q)^2$$

and

$$(6) \quad \frac{\partial F}{\partial q} = \text{Hess } f_{v, \xi} = \sum_{i=1}^m \varphi_i(\xi) \frac{\partial^2}{\partial q^2} \text{dist}(v_i, q)^2.$$

By [17, Lemma 3.11] the matrix $\partial F / \partial q$ is invertible. Hence the derivative $\frac{\partial \Upsilon^{\text{ge}}}{\partial v_i}$ of $\Upsilon^{\text{ge}}(v_1, \dots, v_m; \xi)$ with respect to one of its coefficients v_i can be computed as a minimization problem to obtain the value $\Upsilon^{\text{ge}}(v, \xi)$ and the solution of the linear system of equations

$$\frac{\partial F}{\partial q} \cdot \frac{\partial}{\partial v_i} \Upsilon^{\text{ge}}(v, \xi) = - \frac{\partial F}{\partial v_i}.$$

The expressions $\frac{\partial}{\partial v_i} \frac{\partial}{\partial q} \text{dist}(v_i, q)^2$ and $\frac{\partial^2}{\partial q^2} \text{dist}(v_i, q)^2$ that appear in (5) and (6), respectively, encode the geometry of M . Closed-form expressions for both are given in [15] for the case of M being the unit sphere. For $M = \text{SO}(3)$, the second derivative of $\text{dist}(v, \cdot)^2$ with respect to the second argument has been computed in [18].

3.2. Generalized Jacobi fields as interpolation in the tangent bundle. The isomorphism \mathcal{T} defined in Lemma 3.1 constructs a vector field along a given function Υ from a set of tangent vectors b_1, \dots, b_m at the Lagrange nodes. It can therefore also be interpreted as an interpolation operator for vector fields. Using that the tangent bundle TM can be given the structure of a smooth manifold itself, Hardering showed the elegant result that for variations of geodesic interpolation functions, \mathcal{T} can even itself be interpreted as geodesic interpolation in the sense of Section 2.2, if the metric on TM is chosen appropriately.

The following is taken from [5], Sections 1.2.2 and Remark 2.26. Let $\pi : TM \rightarrow M$ denote the canonical projection. The tangent space of TM at any point (q, V) splits into the horizontal and the vertical subspace

$$T_{(q,V)}TM = H_{(q,V)} \oplus V_{(q,V)},$$

where the vertical subspace is defined as the kernel of $d\pi_{(q,V)}$. Roughly speaking, $H_{(q,V)}$ contains the variations of q , and $V_{(q,V)}$ contains the variations of V .

For any vector $W \in T_qM$ there exists a unique vector $W^h(q, V) \in H_{(q,V)}$ such that $d\pi(W^h) = W$. This vector W^h is called the horizontal lift of W [1], and this lifting defines an isomorphism between T_qM and $H_{(q,V)}$. Likewise, there is a vertical lift W^v of W to $V_{(q,V)}$. For any smooth real-valued function f on M , let $df \in T_q^*M$ be its differential at q , and Wf the derivative of f in the direction of W . There is a unique vector $W^v(q, V) \in V_{(q,V)}$ such that $W^v(df) = Wf$ for all functions f on M . This vertical lift defines an isomorphism between the vector space T_qM and $V_{(q,V)}$.

Using these concepts, we can define a pseudo-metric g^h on TM from the metric g of M . Let (q, V) be a point on TM . Let X_1, X_2, Y_1, Y_2 be elements of T_qM , and $\tilde{X} = X_1^h + X_2^v$ and $\tilde{Y} = Y_1^h + Y_2^v$ be elements of $T_{(q,V)}TM$. The horizontal lift g^h of g on TM evaluated for \tilde{X} and \tilde{Y} is

$$g_{(q,V)}^h(\tilde{X}, \tilde{Y}) = g_q(X_1^h, Y_2^v) + g_q(X_2^v, Y_1^h).$$

It is a pseudo-Riemannian metric on TM of signature (k, k) , with k the dimension of M [10].

Using this apparatus we can show that geodesic vector field interpolation, originally defined by variation of geodesic interpolants, can also be seen as a variational form of geodesic interpolation on TM with respect to the horizontal lift metric. We do not obtain a minimization formulation of geodesic vector field interpolation, as g^h is only a pseudo-metric.

Lemma 3.2 ([5]). *If (v_i, V^i) denotes values in TM , $\Upsilon^{ge}(v, \cdot)$ the geodesic interpolation of the v_i in M , and $\mathcal{T} = \mathcal{T}[V_1, \dots, V_m]$ the interpolation of the V_i in the sense of Lemma 3.1, then we have*

$$\sum_{i=1}^m \varphi_i(\xi) \log_{(\Upsilon^{ge}(v, \xi), \mathcal{T}(\xi))}^h(v_i, V_i) = (0, 0) \in T_{(\Upsilon^{ge}(\xi), \mathcal{T}(\xi))}TM,$$

where $\log_{(q,V)}^h$ is the inverse of the exponential map of the metric g^h at the point (q, V) .

This corresponds to the first-order optimality condition (2) of geodesic interpolation in the tangent bundle TM . If only the projection onto the first factor q is considered the formula degenerates to geodesic interpolation on M .

3.3. Global test function spaces. We now give discretizations of the global test function spaces. They are constructed by piecing together local variations continuously across element boundaries.

Definition 3.2. *Let $u_h \in V_h^M$ be a geometric finite element function. A test function v_h of u_h is a continuous vector field along u_h such that $v_h|_T$ is a (generalized) Jacobi field on $u_h|_T$ for all elements T of \mathcal{G} .*

We note that this definition is equivalent to saying that a test function v_h of u_h is the derivative of a curve in V_h^M at u_h . Therefore, test functions are vectors in the tangent space $T_{u_h} V_h^M$. Indeed, we have:

Lemma 3.3. *Let $u_h \in V_h^M(G)$ be a geometric finite element function, and let $\bar{u} \in M^n$ be its values at the grid vertices. Then $T_{u_h} V_h^M$ is isomorphic to $\prod_{i=1}^n T_{u_i} M$.*

The operator \mathcal{T} defined in Lemma 3.1 extends a set of vectors at the nodal values v_1, \dots, v_m to a vector field along the interpolation function Υ . Given a GFE function u_h , the local operator \mathcal{T} can be generalized naturally to an operator that maps a set of tangent vectors at the nodal values of u_h to a test function along u_h . In an abuse of notation, we will denote both operators by the same letter \mathcal{T} .

Evaluation of global GFE test functions is straightforward. Let η_h be such a function for u_h , and let $x \in \Omega$. Then, to compute $\eta_h(x)$, suppose that T is a grid element with $x \in T$. Then, if ξ are the local coordinates of x in T ,

$$\eta_h(x) = \mathcal{T}[b_1, \dots, b_m](\xi),$$

where b_1, \dots, b_m are the values of η_h at the Lagrange nodes of T . No additional transformation is necessary.

Finally, let u_h be a fixed GFE function. As the space $T_{u_h} V_h^M$ of test functions along u_h is a linear space, it admits a basis representation. In particular, we can even construct a generalization of the nodal basis for $T_{u_h} V_h^M$. Let $T_{u_1} M, \dots, T_{u_n} M$ be the set of tangent spaces at the nodal values of u_h . For each of the spaces $T_{u_1} M, \dots, T_{u_n} M$ select an orthonormal basis, and call the basis vectors ϕ_{ij} , $i = 1, \dots, n$, $j = 1, \dots, \dim M$. To each vector $\phi_{ij} \in T_{u_i} M$ corresponds a test function in $T_{u_h} V_h^M$, defined as the unique function Φ_{ij} in $T_{u_h} V_h^M$ that is equal to ϕ_{ij} at Lagrange node i , and equal to the zero vector on all other Lagrange nodes. The set of all these functions Φ_{ij} , $i = 1, \dots, n$, $j = 1, \dots, \dim M$, forms a basis of $T_{u_h} V_h^M$, which we call the nodal basis. All six test functions shown in Figure 3 are such nodal basis functions.

4. EQUIVALENCE IN THE CASE OF MINIMIZATION PROBLEMS

In the original presentation of geodesic finite element functions [15], only PDEs with a minimization formulation were considered. The definition of discrete test function spaces was avoided by moving directly to an algebraic minimization problem. First and second variations were hence only ever taken in the algebraic setting, where it was clear that $\prod_{i=1}^n T_{v_i} M$ is the proper space of variations around an algebraic configuration $\bar{v} \in \mathcal{M} \subset M^n$, $\bar{v} = (v_1, \dots, v_n)$.

Now that discrete test function spaces are available, it is possible to also consider optimality conditions for minimization problems in the spaces of GFE functions. In this section we show that, with the definition of test functions given in this paper, these two approaches are equivalent. In other words, we show that the following diagram commutes:

$$\begin{array}{ccc}
V_h^M & \xrightarrow{d} & TV_h^M \\
\mathcal{E} \downarrow & & \downarrow \mathcal{T}^{-1} \\
M^n & \xrightarrow{d} & TM^n
\end{array}$$

The proof is short and the result may be obvious for people skilled in geometric analysis. We show it nevertheless for readers with other backgrounds.

Let $\mathcal{J} : H^1(\Omega, M) \rightarrow \mathbb{R}$ be a sufficiently smooth energy functional. We want to find approximate minimizers of this functional using the geometric finite element method. For this, we first restrict \mathcal{J} to the discrete geometric finite element function space V_h^M . This is possible without any approximation error as the GFE spaces are subsets of H^1 (Theorem 2.3).

At this point, there are two ways to proceed. The approach chosen in [15] identifies the discrete space V_h^M with the algebraic space $\mathcal{M} \subset M^n$ (locally). This leads to the algebraic minimization problem in \mathcal{M} (locally) for the functional

$$J : \mathcal{M} \rightarrow \mathbb{R}, \quad J(\bar{v}) := \mathcal{J}(\mathcal{E}^{-1}(\bar{v})).$$

A necessary condition for $\bar{v} \in \mathcal{M}$ to be a minimizer of J is that the first variation of J at \bar{v} vanishes

$$(7) \quad dJ[\bar{v}](\bar{\eta}) = 0 \quad \forall \bar{\eta} \in T_{\bar{v}}M^n.$$

This is the path through the lower left corner in the diagram above.

The second formulation uses discrete test functions to state the first-order optimality conditions directly in the discrete function space. A necessary condition for v_h to be a local minimizer of \mathcal{J} in V_h^M is that the first variation vanishes. Suppose that the test functions we have defined in Section 3 are defined in the correct way. Then, a necessary condition for v_h to be a local minimizer of \mathcal{J} in V_h^M is that the derivative of \mathcal{J} is zero in the direction of all test functions η_h

$$d\mathcal{J}[v_h](\eta_h) = 0 \quad \forall \eta_h \in T_{v_h}V_h^M.$$

Using the evaluation operators \mathcal{E} and \mathcal{T}^{-1} for GFE functions and test functions, respectively, we can obtain an algebraic form of this optimality condition

$$(8) \quad d\mathcal{J}(\mathcal{E}^{-1}(\bar{v}))(\mathcal{T}(\bar{\eta})) = 0, \quad \forall \bar{\eta} \in T_{\bar{v}}M^n.$$

This is the path through the upper right corner in the diagram above.

The following result states that both paths are equivalent. This is the justification for our definition of test functions.

Theorem 4.1. *Problems (7) and (8) are equivalent.*

Proof. Suppose that $\bar{v} \in M^n$ is such that

$$dJ[\bar{v}](\bar{\eta}) = 0$$

for any $\bar{\eta} \in T_{\bar{v}}M^n$. This means that for any $\bar{\eta}$ there is a curve $C : (-\epsilon, \epsilon) \rightarrow M^n$ with $\dot{C}(0) = \bar{\eta}$ such that

$$\left. \frac{d}{dt} \mathcal{J}(\mathcal{E}^{-1}(C(t))) \right|_{t=0} = 0.$$

Let $c := \mathcal{E}^{-1}(C(\cdot))$ be the corresponding curve in V_h^M . Then

$$\begin{aligned} 0 &= \frac{d}{dt} \mathcal{J}(c(t)) \Big|_{t=0} \\ &= d\mathcal{J}(c(0)) \left[\frac{dc}{dt} \Big|_{t=0} \right] \\ &= d\mathcal{J}(v_h)[\eta_h] \\ &= d\mathcal{J}(\mathcal{E}^{-1}(\bar{v}))(\mathcal{T}(\bar{\eta})), \end{aligned}$$

which is (8). As the same argument also works backwards, both formulations are equivalent. \square

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